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Formation of grain boundaries in ductile single crystals at finite plastic deformations

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The paper is dedicated to the 60th birthday of M. Ortiz.

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ABSTRACT

The theory of formation of grain boundaries in ductile single crystals is proposed within the nonlinear continuum dislocation theory (CDT), where grain boundaries are interpreted as surfaces of weak discontinuity in placement but strong discontinuity in plastic slip. The set of governing equations and jump conditions are derived for the energy minimizers admitting such surfaces of discontinuity from the variational principle. By constructing energy minimizing sequences having piecewise constant plastic and elastic deformation in two examples of ductile single crystals deforming in plane strain simple shear or uniaxial compression, it is shown that the formation of lamellae structure with grain boundaries is energetically preferable. The number of lamellae is estimated by minimizing the energy of grain boundaries plus the energy of boundary layers.

1. Introduction

During various cold working processes producing severe plastic deformations like traditional rolling, drawing, extrusion, or newly invented equal channel angular pressing (Segal, 1999; Valiev and Langdon, 2006) and high pressure torsion (Vorhauer and Pipan, 2004; Sakai et al., 2005) (see also the review paper written by Valiev et al. (2000) and the references therein), metals and alloys undergo significant microstructural changes. Among such changes one should mention the formation and evolution of grain and subgrain boundaries (Kuhlmann-Wilsdorf and Hansen, 1991; Hughes and Hansen, 1997), deformation twinning in low stacking fault metals and alloys (Tome et al., 1991; Christian and Mahajan, 1995), formation of macroscopic shear bands in polycrystals (Jia et al., 2003) and single crystals (Harren et al., 1988; Uchic et al., 2009) et cetera. The structural changes of metals and alloys at microlevel may influence the macroscopic properties of these materials directly, as the Taylor and Hall–Petch relations show (see, for instance, (Hansen, 2004; Jiang and Weng, 2004)). As a consequence, new materials with exceptionally high strength could be created in this way. Therefore, the following question, interesting from the theoretical and important from the practical point of view, arises: what kind of theory can we develop to explain and predict such microstructural changes as well as the accompanying macroscopic responses of the materials? Unfortunately, so far there is no comprehensive answer to this question except for some particular cases. However, one thing is for sure: since the plastic slip as the product of collective movement of a huge number of dislocations and grain boundaries

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are the active participants in this structural rearrangement during cold working processes, any physically meaningful theory of formation and evolution of microstructure should capture their behavior in a proper way.

One of the main guiding principles in seeking an appropriate theory of formation of microstructure in metals and alloys has first been proposed by Hansen and Kuhlmann-Wilsdorf (1986) in form of the so-called LEDS-hypothesis: the dislocation structures in the final state of deformation minimize the energy of crystals (see also (Laird et al., 1986; Kuhlmann-Wilsdorf, 1989)). However, it is still difficult to develop the theory of formation of dislocation structures based on this principle alone. The crucial step in this direction has been done by Ortiz and Repetto (1999), and Ortiz et al. (2000), who introduced a new ingredient to the energy minimization, namely the non-convexity of the energy. In their papers the problem of non-convex energy minimization has been formulated and studied for ductile crystals within the finite crystal plasticity. By observing that the pseudoelastic energy densities of crystals undergoing geometrical softening or latent hardening are in fact non-convex, they showed that the laminate structures in which the piecewise constant plastic deformation caused by a single slip system and the piecewise constant elastic deformation in form of pure rotation serve as the energy minimizing sequences. Later on, Carstensen et al. (2002) discovered the non-convexity of the energy densities even for crystals deforming in single slip without geometrical softening or latent hardening and thus, extended the non-convex energy minimization to the whole finite crystal plasticity. But crystal plasticity, as a phenomenological theory, operates with plastic slips while ignoring their source: dislocations. To achieve an agreement with experiments it has to introduce several phenomenological concepts like back stress or hardening as internal variables obeying additional constitutive equations which would otherwise be derivable as natural consequences of a more general continuum dislocation theory (see the series of our papers (Berdichevsky and Le, 2007; Le and Sembiring, 2008a,b, 2009; Kochmann and Le, 2008a,b, 2009; Kaluza and Le, 2011; Le and Nguyen, 2012, 2013), as well as the alternative approaches in (Lee et al., 2010; Lim et al., 2011; Engels et al., 2012; Öztop et al., 2013; Mayeur and McDowell, 2014)). Let us mention also an approach proposed recently by Zhu et al. (2013); Zhu and Xiang (2014) in which continuum models of dislocation densities on low angle grain boundaries and the grain boundary energy (including also the long-range elastic energy when the grain boundary is not in equilibrium) are derived from the discrete dislocation dynamics. Such approach has the advantage of capturing details of the formation process of grain boundaries in which the grain boundaries are in general non-equilibrium. Ortiz and Repetto (1999), at the end of their paper, did include the dislocations and their energy into the crystal plasticity to justify some heuristic estimates for the spacing of the dislocation walls and pointed out the way of generalization to the continuum dislocation theory. However, to the best of our knowledge, the whole set of governing equations as well as the boundary and jump conditions that must be satisfied at the grain boundaries have not yet been derived and studied thoughtfully from the continuum dislocation theory.

The aim of this paper is twofold. First, we want to extend the nonlinear continuum dislocation theory (CDT) developed recently by Le and Günther (2014) to the case of crystals containing newly formed grain boundaries. Regarding grain boundaries as surfaces of weak discontinuity in placement but strong discontinuity in plastic slip, we include the energy of such boundaries into the energy functional of the crystal and study the variational problem of minimizing the energy of crystal containing dislocations and grain boundaries. We derive from this variational problem the whole set of equilibrium equations, boundary conditions, and jump conditions at the grain boundaries. It turns out that the grain boundaries will stay in equilibrium if and only if the thermodynamic driving force, including also the curvature of the jump surface, vanishes. This explains why the microstructure obtained in the final state of deformation must be lamellar. Second, we apply the developed theory to two plane strain problems for single crystal deforming in single slip under the condition of simple shear or uniaxial compression. Due to the non-convexity of the energy in certain ranges of the overall shear or stretch, the construction of the lamellae with piecewise constant plastic and elastic deformation leads to the energy minimizing sequences as the solutions of these non-convex variational problems. In case of plate under uniaxial compression the uniform states are not rank-one connected, so dislocations and grain boundaries should adapt to the elastic strains chosen from the homogeneous states in a smart way to satisfy the compatibility condition and, at the same time, to minimize the energy. It turns out that the whole set of jump conditions is needed to determine the orientation of grains (which are misoriented with respect to the slip direction), the plastic slips, and the elastic rotations.

The paper is organized as follows. After this short introduction we present in Section 2 the main ingredients of the nonlinear CDT. Section 3 extends this nonlinear theory to the case of crystal with grain boundaries. Section 4 formulates the plane strain problems. Sections 5 and 6 are devoted to the problem of single crystal deforming in constrained simple shear and uniaxial compression, respectively. Finally, Section 7 concludes the paper.

2. Nonlinear continuum dislocation theory

Nonlinear CDT starts from the basic kinematic resolution of the deformation gradient $\mathbf{F} = \partial\mathbf{y}/\partial\mathbf{x}$ into elastic and plastic parts (Bilby et al., 1957)

$$\mathbf{F} = \mathbf{F}^e \cdot \mathbf{F}^p. \tag{1}$$

We attribute an active role to the plastic deformation: $\mathbf{F}^p$ is the deformation *creating* dislocations (either inside or at the boundary of the volume element) or *changing* their positions in the crystal without distorting the lattice parallelism (see Fig. 1). In contrary, the elastic deformation $\mathbf{F}^e$ deforms the crystal lattice having *frozen* dislocations (Le and Günther, 2014).